APTIM

Draft
Hydrus Modeling Work Plan
Former George Air Force Base
Victorville, California

Air Force Civil Engineer Center
2261 Hughes Avenue, Suite 163
Lackland AFB, Texas 78236

Prepared by:
APTIM
2410 Cherahala Boulevard
Knoxville, Tennessee 37932

Contract No. FA8903-09-D-8580, Task Order 0018
Project No. 145981
Revision 0
April 2018

Draft
Hydrus Modeling Work Plan
Former George Air Force Base
Victorville, California

Contract No. FA8903-09-D-8580
Task Order 0018

Revision 0
April 2018

Gary R. Hecox, PhD Primary Author	Date
Homayoun (David) Daftary, PG, CHG Project Manager	Date

Table of Contents

List of Figures

List of Tables

Acronyms and Abbreviations

Acronym	**Reference**
1-1/n	van Genuchten m (unitless)
2D	Two-dimensional
3D	Three-dimensional
α	van Genuchten curve fit alpha (1/cm)
API	American Petroleum Institute
Aptim	Aptim Federal Services LLC
CIMIS	California Irrigation Management Information System
cm	Centimeter
D^{air}	Molecular diffusion coefficient in air (cm^2/sec)
D^{eff}	Effective molecular diffusion coefficient in vapor (cm^2/sec)
D^{w}	Molecular diffusion coefficient in water (cm^2/sec)
ESL	Environmental Screen Level
GAFB	George Air Force Base
GIS	Geographical information system
H'	Unitless Henry's Law constant
h_c	Capillary pressure, pressure head for vapor-water systems (cm water)
$K(h_c)$	Hydraulic conductivity at given pressure head/water saturation (cm/d)
Koc	organic carbon partitioning coefficients
K_s	Saturated hydraulic conductivity (cm/d)
LNAPL	Light Non-Aqueous Phase Liquid
$\mu g/cm^3$	micrograms per cubic centimeter
n	van Genuchten curve fit n (unitless, referred to as the *beta* parameter in some references)
θ_T	Total porosity (fraction)
θ_v	Vapor (air)-filled porosity (fraction)
θ_v	Water-filled porosity (fraction)
S_{ew}	Effective saturation of water at given capillary pressure (fraction)
S_w	Total water saturation (fraction)
S_{wir}	irreducible water saturation (fraction)
USCS	Unified Soil Classification System
voxel	3D volumetric grid element

EXECUTIVE SUMMARY

This work plan presents the procedures and data used to develop Hydrus variably saturated flow and transport finite element models for various sites at former George Air Force Base (GAFB). As to be implemented at GAFB, Hydrus models will be set up as a two-dimensional vertical profile model across the selected model area.

A Hydrus model is based on the lithology along a vertical cross-section through the highest concentrations of a vapor and/or groundwater plume. This cross-section is developed from the 3D lithologic data model for a site based on Unified Soil Classification System (USCS) soil types. GAFB site-specific geotechnical soil test results, classified by lithology, will be used to define the flow and transport variable parameter values for the various types of soils along the lithologic cross-section. Parameters defined by soil type are hydraulic conductivity, porosity, bulk density, fraction of organic carbon, distribution coefficient, and van Genuchten parameters. Ten capillary pressure test results are available for the GAFB well- and poorly-graded sandy soils. These results will be augmented by published van Genuchten parameter values for various soil types. Additional Hydrus model inputs are the 20 years of daily precipitation and evaporation data from California Irrigation Management Information System (CIMIS) station 117 from the CIMIS online database and compound specific transport parameters from the San Francisco Regional Water Quality Control Board (2016) environmental screening table IP-1.

Artificial recharge operations have and continue to have substantial impacts on Upper and Lower Aquifer groundwater flow directions, gradients, and contaminant migration. As such, artificial recharge rates or the impact of those rates will be incorporated into the majority of the Hydrus models for the various sites across former George Air Force Base. Temporal pond discharge and irrigation application data have been compiled and will be used to determine artificial recharge rates for the respective artificial recharge areas.

The flow portion of a Hydrus model will be calibrated to observed water level changes over time. Calibration of the transport portion of a Hydrus model will be the evolution of a contaminant plume from ground surface to the presently observed plume extents. Both vadose zone and groundwater plumes will be simulated. Primary calibration variables were hydraulic conductivity, artificial recharge rates from various sources (natural recharge is calculated internally in Hydrus from the daily precipitation/evapotranspiration input data), initial source concentrations and flux, dispersion coefficients, vapor diffusion coefficients, and degradation rates. Both flow and transport calibration will use observed time-series data as calibration targets.

A standard report format for each site modeled will be used for documenting a Hydrus model setup, calibration, and results. The reported results will depend on the objective of the Hydrus model with the majority of the Hydrus model results related to site remediation and closure.

1.0 INTRODUCTION

The objective of this work plan is to define the procedures for the application of the Hydrus 2D/3D variably-saturated groundwater flow and transport model code (Šimůnek et al., 2016; Šimůnek et al., 2013) to various sites at the former George Air Force Base (GAFB; **Figure 1**) for purposes of defining remediation goals and soil cleanup criteria. This work plan addresses Hydrus model input data, model setup, and flow and transport calibration.

In the original work plans, it was proposed to use either SESOIL (Bonazountas and Wagner, 1981, 1984) or VLEACH (Ravi and Johnson, 1997). SESOIL is a deterministic model that uses algebraic equations to generate a result. SESOIL was developed such that no calibration is required (Bonazountas and Wagner, 1981, 1984, p. 2-4). SESOIL originally had substantial mass-balance errors that have been corrected in the commercial license version 7.1. The original public domain version of SESOIL is no longer available for this reason. VLEACH is a finite-difference numerical code that uses simple discretization of a vertical soil column to determine contaminant flux to the water table. A comparison of the two models can be found at (ESCI, 2003). During review of available software programs, Hydrus 2D/3D (described below) was selected for the following reasons:

1. Hydrus simulates the wetting and drying of the vadose zone soil column and associated change in hydraulic conductivity that is associated with changing water content as soils wet and dry. This is a critical function in vadose zone contaminant transport (Radcliff and Šimůnek, 2010). SESOIL and VLEACH do not have this capability.
2. Hydrus uses saturated hydraulic conductivity as one of the basic input parameters for solving the groundwater flow and transport equations. In the vadose zone, saturated hydraulic conductivity is adjusted as a function of water content using the van Genuchten equations (van Genuchten, 1980). VLEACH does not include hydraulic conductivity in the equations used but instead calculates water flux as a function of recharge rate and porosity. SESOIL does not incorporate variations in hydraulic conductivity as a function of water content.
3. Hydrus uses daily evapotranspiration and precipitation along with wetting and drying of the underlying soils to calculated recharge to the water table. VLEACH does not use meteorological data to determine recharge but instead requires a user input value. SESOIL calculates recharge using monthly precipitation and daily evapotranspiration data using a mass-balance equation. VLEACH and SESOIL do not incorporate daily changes in evapotranspiration as a result of storm precipitation in a manner similar to Hydrus.
4. Hydrus has internal computational protocols to control time-steps and thus minimize Courant numbers and has setup tools to minimize Peclet number to control numerical dispersion. VLEACH is a finite difference code with no allowance for numerical dispersion control that can result in large over-prediction of contaminant transport velocities. SESOIL is "compartmental" balance model that is independent of the size

and shape of the soil column (Bonazountas and Wagner, 1981, 1984, p 1-5) and thus does not have to address numerical stability.

5. Hydrus incorporates various changes in lithology for horizontally and vertically as discussed in Section 3. SESOIL and VLEACH code do not allow for vertical lithologic changes in the vadose zone soil column.
6. As implemented for GAFB, Hydrus includes simulation of contaminant migration through the vadose zone into underlying groundwater with subsequent groundwater migration in the Upper and Lower Aquifers. SESOIL and VLEACH do not address groundwater transport below the vadose zone. For these two codes, groundwater transport has to be addressed using a separate modeling program.

1.1 Description of Hydrus Model Code

Hydrus-2D/3D (Šejna et al., 2011; Šimůnek et al., 2012; Šimůnek et al., 2016; Šimůnek et al., 2013; Yu and Zheng, 2010) can simulate flow and contaminant transport in variably-saturated porous and fractured media including diffusion, volatilization, dispersion, retardation, and degradation transport processes. Hydrus uses internal control to maintain Peclet and Courant numbers (Zheng and Bennett, 1995) within model stability criteria and limit numerical dispersion. The Peclet number is a measure of the finite element size divided by the dispersion coefficient and is minimized to control numerical oscillations. The Courant number is a measure of the time step size in relation to the finite element size and groundwater flow velocity and is minimized to control numerical dispersion.

Contract No. FA8903-09-D-8580, Task Order 0018• Draft • Revision 0 • April 2018 •

To perform a meaningful GAFB transport simulations under time-variable partially-saturated flow boundary conditions, such as episodic precipitation events, frequently requires Hydrus to use time steps in the one to ten second range. For a typical GAFB 20-year two-dimensional (2D), 20,000 element simulation, between 50,000 and 100,000 complete model iterations are required for a single simulation. It is also noted that contaminant migration from ground surface through the vadose zone into the Upper and Lower Aquifers is a critical component to understanding and simulating contamination at GAFB and developing meaningful soil and groundwater remediation goals.

1.2 GAFB Hydrus Model Structure

For GAFB remedial evaluations, Hydrus models will be developed for individual sites as described in Section 3. For a given site such as OU5 SS083, Hydrus will be set up as a 2D vertical profile model in the horizontal (X) and vertical (Z) planes. Hydrus models will be set up in consistent units of centimeters, days, and concentration units of micrograms per cubic centimeter ($\mu g/cm^3$, equivalent to mg/L). Hydrus models will simulate water and contaminant transport assuming equilibrium partitioning between the vapor, water, and soil phases.

In Hydrus, contaminant input and output is defined in terms of water concentrations that can readily be converted to vapor or soil concentrations using partitioning equations. Groundwater, soil, and vapor contamination will be related using Henry's Law and organic carbon partitioning constants from the Environmental Screen Level (ESL) documents compiled by the San Francisco Regional Water Quality Control Board (2016). Site-specific porosity values, organic carbon concentrations, and bulk densities will be used to calculate distribution coefficients and resulting retardation factors. Note that Hydrus can simulate non-equilibrium partitioning contaminant transport such as for the dieldrin groundwater plume at Site OT071.

1.3 Modeling Objectives for CERCLA and Non-CERCLA Sites

The Hydrus model objectives are:

1. Hydrus model results will be used as one of the lines of evidence supporting closure of selected sites.
2. Assess contaminant migration and attenuation from source areas through the vadose zone into underlying groundwater and subsequent groundwater contaminant migration. For example, because Hydrus uses basic data such as daily precipitation and evapotranspiration to calculate recharge through the vadose zone, the resulting recharge rate is likely to be more representative of actual site conditions compared to assuming there is no natural recharge based on annual precipitation and evapotranspiration data (MWH Americas, 2011).
3. For vadose zone sites, determine soil cleanup concentrations to protect underlying groundwater and achieve site closure. Since soil vapor concentrations are readily available from the monitoring programs, cleanup concentrations will be expressed as equilibrium concentrations for both soil and vapor.
4. For sites with a groundwater plume below the vadose zone, calculate vadose zone vapor concentrations resulting from a migrating groundwater plume. This is important for soil site closure because, for a site such as SS083, the underlying groundwater plume is likely contributing the bulk of the contaminant mass currently being removed by the soil vapor extraction system.
5. Evaluate vapor and groundwater contaminant migration from the LNAPL at sites SS030 and ST067b. Hydrus will be used with LNAPL migration/remediation codes such as LNAST (API, 2004) or LDRM (Charbeneau, 2007; Charbeneau and Beckett, 2007) to address LNAPL migration and remediation alternatives for these sites. The same lithology hydraulic parameters will be used for both the Hydrus and LNAPL modeling.
6. Evaluate remedial options for vadose zone and groundwater contamination at sites SS030, ST067b, OT069, and OT071.
7. For dieldrin site OT071, assess various transport mechanisms that could account for dieldrin migration from the sites of application at ground surface into Upper and Lower Aquifer groundwater.

2.0 INPUT DATA FOR HYDRUS MODELS

This section describes the basic data compilation and processing required for developing a Hydrus model. Setup and calibration of a Hydrus model, using SS083 as an example, is described in Section 3.0.There are a number of datasets required for development of a Hydrus flow and transport model for a GAFB site. These include:

- Meteorological precipitation and evapotranspiration data over time
- Geotechnical parameter values for each lithologic type including variable-saturation van Genuchten parameters
- Hydraulic conductivity values
- Compound-specific transport parameters
- Vapor and groundwater concentrations over time
- Groundwater levels over time
- Artificial recharge locations. While the volume of water discharged to a feature such as a pond is helpful in determining groundwater recharge rates, the complexity of recharge is such that the actual recharge rates will be a calibration variable to calibrate the model to water levels over time.
- Detailed lithology from ground surface into the Lower Aquifer

2.1 Model Input Parameters

The input parameters for a GAFB Hydrus model are:

- **Artificial recharge.** Groundwater systems at GAFB have been or continue to be impacted by various artificial recharge operations. These operations have resulted in changes to flow direction, flow gradient and velocities, and contaminant migration from source areas. The artificial recharge operations that will be incorporated into the applicable Hydrus models are:
  - Adelanto Sewage Treatment ponds (Adl. STP, Sept 1998 - Present)
  - Ball Fields (1961?-present)
  - Base Housing area (1961-1994)
  - Golf Course area (1964-Present)
  - Golf Course Pond (GCP, 1964-present)
  - New Percolation Ponds (NPP, Oct 1996 - March 2003)
  - Schmidt Park (1961?-present)
  - Old Sewage Treatment Plant ponds (Old STP, Dec 1991- Oct 1996)
  - Victor Valley Water Reclamation Authority ponds (VVWRA, 2001-present).

- **Meteorological data**. Twenty three years of daily precipitation and evapotranspiration meteorological data (1994-2017) from the California Irrigation Management Information System (CIMIS) online database (California Dept. of Water Resources, 2017) Victorville station 117 are used as input values for the upper atmospheric pressure boundary of the model (**Figure 2**). It was assumed that plant water uptake and transpiration are negligible. Hydrus is limited to 15,000 daily meteorological data records so this observed dataset is repeated for simulations outside of the1994-2017 date range. For example, a calibration simulation from 1948 to 2017 (69 years) would use the meteorological dataset three times.

- **Soil geotechnical parameters**. Bulk density, porosity, moisture content, grain-size, fraction of organic carbon, and hydraulic conductivity results from 81 geotechnical tests conducted on GAFB soil samples were compiled into a database. The soil type for each test result was determined using associated grain-size analyses. For the few samples that did not have an associated grain-size analysis, the soil type was determined using the descriptions from the boring logs. Pertinent statistical summary results are tabulated by soil type on **Table 1** with histograms of selected parameters on **Figure 3.** Mean values define initial parameter values and ranges determined upper and lower parameter limits for the various soil types in the Hydrus model.

- **Variable saturation soil parameters**. The van Genuchten/Mualem (Mualem, 1976; van Genuchten, 1980) soil-hydraulic model was selected in Hydrus to define the relationship between soil moisture content, capillary pressure, and hydraulic conductivity. van Genuchten parameters are determined from capillary pressure tests and define the non-linear relationship between hydraulic conductivity and fluid saturation (Šimůnek et al., 2012, p. 15-16) for each soil type. In model computations these parameters control the changes in hydraulic conductivity over time as precipitation-related recharge pulses migrate through the vadose zone defined by the following equations (Šimůnek et al., 2012; van Genuchten, 1980):

$$S_{ew} = \left[\frac{1}{1+(\alpha h_c)^n}\right]^m = \frac{S_w - S_{wir}}{1 - S_{wir}}$$

$$K(h_c) = K_s\left(S_{ew}^{1/2}\left[1-\left(1-S_{ew}^{1/m}\right)^m\right]^2\right)$$

where

S_{ew} = effective saturation of water at given capillary pressure (fraction)
S_w = total water saturation (fraction)
S_{wir} = irreducible water saturation (fraction)
h_c = capillary pressure, pressure head for vapor-water systems (cm water)
α = van Genuchten curve fit alpha (1/cm)
n = van Genuchten curve fit n (unitless, referred to as the *beta* parameter in some references)
m = 1-1/n (unitless)
$K(h_c)$ = Hydraulic conductivity at given pressure head/water saturation (cm/d)
K_s = Saturated hydraulic conductivity (cm/d for GAFB Hydrus models)

Ten capillary test results are available for GAFB soil samples. These tests were conducted on GAFB samples collected for the Light Non-Aqueous Phase Liquid (LNAPL) migration analysis (IT Corporation, 1998). As shown on **Table 2**, the samples are from well-graded (SW) and poorly-graded (SP) sandy soils with one test each on silt, silty sand, and gravel soils.

To augment these site-specific results, van Genuchten parameter values for the various GAFB soil types were evaluated from the American Petroleum Institute (API) LNAPL database (Beckett and Joy, 2006) that contains results from approximately 250 capillary pressure tests on a wide-range of soil types (**Table 3**). van Genuchten values from the site-specific tests augmented by those in **Table 3** were used as parameter values in the Hydrus model soils. Comparison of the site specific and API average van Genuchten alpha and n (beta) values by soil type are presented on **Table 4**.

Figure 4 illustrates the relationship between the limited number of site-specific capillary test results and those from the more extensive API database. As illustrated, the values of the van Genuchten parameter n (or beta) is relatively insensitive to changes in soil types. The van Genuchten parameter α, is sensitive to changes in lithology, varying by approximately a factor of 10 from clay to gravel.

Note that van Genuchten parameters do not affect flow and transport in fully saturated soil as the capillary pressure, h_c, would be zero for this condition and S_{ew} would be equal to 1 in the equations above.

- **Hydraulic conductivity.** A comprehensive evaluation of GAFB hydraulic conductivity data is presented in the SS030 LNAPL Conceptual Site Model Report (CB&I Federal Services (2017) and summarized herein. Hydraulic conductivity values from 70 site-specific laboratory and 91 field pumping and slug tests were evaluated for purposes of developing Hydrus models. As shown on **Figure 5**, classified by soil type, site-specific laboratory test results tend to be about an order of magnitude less than the average values from the API database but the upper/lower 95% mean value error bars tend to be larger. **Figure 6** presents histograms of horizontal and vertical hydraulic test results from field slug and pumping tests and **Table 5** presents summary statistics by unit, test type and horizontal and vertical hydraulic conductivity results. **Figure 7** presents a comparison between field aquifer and laboratory tests.

As shown, laboratory test results are about an order of magnitude less than overall field test results and slug test values tend to be about an order of magnitude less than pumping test values. For Hydrus modeling, it is necessary to define parameters based on lithology. It has proven to be problematic to classify the field aquifer tests by lithology type while the majority of the laboratory tests had accompanying grain-size analysis making lithologic classification straight-forward. To address the bias between the laboratory and field hydraulic conductivity values, for the modeling in this work plan, it is recommended that, where available, the GAFB upper 95% mean back-transformed values on **Table 4** be used for initial hydraulic conductivity values for each lithology type. For example, for SP sands, the initial hydraulic conductivity value will be 6.3 x 10-3 cm/sec (20 ft/d).

The exception to this is in the deeper coarse sands of Lower Aquifer where only a few laboratory test results are available. For these sands, hydraulic conductivity values from water supply well pumping tests will be used as the initial values. These values are in the range of 0.05 to 0.10 cm/sec (100 to 200 ft/d).

- **Compound-specific contaminant transport parameters.** Compound specific contaminant transport parameters from the San Francisco Regional Water Quality Control Board (2016) environmental screening table IP-1 will be used for the Hydrus modeling. This includes organic carbon partitioning coefficients (Koc), Henry's constants, molecular weights, and free air and water diffusion coefficients. The Millington/Quirk tortuosity model (Johnson, 2002, Eq. 2; Millington and Quirk, 1961; Šimůnek et al., 2012; Eqs. 3.47-3.49) will be used calculate effective porous media vapor diffusion coefficients for the compounds of concern. The effective vadose zone effective diffusion coefficient is defined by Johnson-Ettinger vapor intrusion equation (Johnson, 2002, Eq. 2) as follows:

$$D^{eff} = D^{air} * \left(\frac{\theta_v^{3.33}}{\theta_t^2}\right) + \left(\frac{D^w}{H'}\right) * \left(\frac{\theta_w^{3.33}}{\theta_t^2}\right)$$

where

D^{eff} = effective molecular diffusion coefficient in vapor (cm2/sec)
D^{w} = molecular diffusion coefficient in water (cm2/sec)
D^{air} = molecular diffusion coefficient in air (cm2/sec)
θ_T = total porosity (fraction)
H' = unitless Henry's Law constant
θ_v = vapor (air)-filled porosity (fraction)
θ_w = water-filled porosity (fraction)

2.2 3D Data Modeling

Lithology type and associated geotechnical characteristics are the foundation upon which the Hydrus models will be constructed. In addition, vapor and groundwater contaminant plume migration over time and present extent will be the Hydrus transport calibration parameters. The primary sources of detailed lithology data are boring and geophysical logs from the hundreds of borings across GAFB while the source of the vapor and groundwater contaminant data is the geographical information system (GIS) database containing data from the early 1990's (as available) to present. Both the lithologic and concentration data are processed using 3D data modeling methods as described below following the data processing steps shown on **Figure 8**. Aptim uses RockWorks 17 (Rockware, 2017) for this modeling but the following steps are typical of an overall 3D data modeling process. Data from SS083 are used in the example below.

1. Data distributions are evaluated both horizontally (**Figure 9**) and vertically (**Figure 10**) and the model area and vertical extent defined. At this step, data are reviewed for obvious anomalies or errors and the horizontal and vertical grid spacing values

determined. Horizontal grid spacings are usually either 25 or 50 feet and vertical grid spacings are 2 or 5 feet. Grid spacing size is dependent on the size of the model area that in turn determines the computational resources required for the 3D gridding. Typically, 3D models of between 10 and 20 million voxels (the term for 3D grid cells) are preferred based on computer resources but occasionally, models of 30 million voxels are created for models that cover the entire GAFB area.

2. Topographic and water table surfaces from the GIS are imported into RockWorks and subsampled to the given model area defined in Step 1 (**Figure 11**). These provide grid control surfaces for the 3D data modeling. For example, ground surface provides the upper boundary for vapor and lithology modeling and Upper Aquifer water table surface provides a lower boundary for 3D vapor modeling and the upper boundary for groundwater plume 3D modeling.
3. The 3D data models are created in RockWorks. Different algorithms are used depending on the type of model being developed (**Figure 12**).
   a. The RockWorks lithoblend algorithm is used for lithology modeling. This algorithm was developed to limit sharp changes in lithology and is only used for lithologic modeling.
   b. The 3D inverse distance weighted algorithm is used for concentration data
      i. Horizontal exponents between 1 and 2 and vertical exponents between 4 and 6 are used. The higher the exponent, the more localized the gridded concentrations around a given data point will be.
      ii. For most concentration gridding, logarithmic data values are used as grid input values. Transformation of the original data into logarithmic values and back-transformation of the 3D grid to normal values is handled by the RockWorks gridding algorithms.
      iii. Other options are declustering for closely-spaced data, resampling of widely-spaced vertical data, and grid cutoff distances for widely-space horizontal data.
      iv. Applicable control surfaces are incorporated as noted in Step 2.
4. Model results are reviewed for consistency with observed data and overall plume configuration.
5. Minor adjustments to the grid parameters are made as necessary and the data are regridded. Depending on the data distribution, data may be regridded two or three times to obtain a realistic final 3D model.

Once the 3D data models are developed, composite data models consisting of the various surfaces and plumes (**Figure 13**), plan maps (**Figure 14**) and cross sections (**Figure 15**) are developed for use in setting up the Hydrus model. A cross-section through the areas of highest vapor and groundwater concentrations will be used for the Hydrus model input lithology.

2.3 Time-Series Data Evaluation

The Hydrus model will use transient flow and transport calibration procedures. Therefore, time-series graphs are generated for both water level and vapor and groundwater concentration data (**Figure 16**). In the Hydrus transport calibration, the simulated water levels and concentrations will be plotted with the observed concentrations on the same graph. Because Hydrus outputs water levels in terms of pressure heads, observed water level data will be converted to equivalent pressure heads with the water table set at a pressure head of zero.

3.0 MODEL SETUP AND CALIBRATION

The basic data discussed in Section 2.0 is used to setup and calibrate a Hydrus model as described in the following sections. The model setup addresses the basic structure of the model such as lithology and boundary conditions. Calibration addresses adjustment of model parameters to generate output that is compared to observed data. The example for this work plan is a model of Operable Unit (OU) 5 Site SS083.

3.1 Model Setup

Hydrus models can be developed solely by creating a finite element mesh and assigning hydrogeologic properties to individual elements of the mesh. However, the standard method of creating a finite element model by manual input of hydrogeologic features by editing individual mesh elements for a large model containing 10,000+ elements is laborious and makes quality control difficult.

For these reasons, Hydrus 2D/3D implements a method for creating the finite element mesh and assigning properties using geometric polygons, lines, or points. These geometric features control mesh generation and allow for relatively easy quality control for the model. This method is combined with local mesh editing to generate the final finite element mesh. This method also makes it easier to incorporate model changes during calibration. This combination method will be used to create the GAFB Hydrus models.

For GAFB, Hydrus models will be setup using the follow procedure:

1. Cross-sections are created through the 3D lithology and plume data models to serve as the template for construction of the Hydrus model. These cross-sections include well screen and applicable surfaces (**Figure 17**). The vapor and groundwater plumes serve for source areas reference and to compare to the Hydrus model output. The cross-sections are exported to bitmaps then imported and referenced to the Hydrus grid to serve as base sections for the model setup. Plume configurations are used only for defining source areas and spatial references for simulation setup. Observed plumes are, however, not input into the model as initial conditions. For the start of a calibration simulation, initial concentrations are set to zero.
2. The bitmap sections are used as templates for defining Hydrus geometric objects. Each object represents a lithologic unit, monitor well screen location, model boundary, or a mesh refinement area (**Figure 18**). Geometric objects control how the finite element mesh is created and are not changed when the mesh is generated. Each node on a geometric object will also be a node in the mesh. This makes it easy to locate objects such as observation nodes at well screens or flow particles at key locations.
3. The geometric features are used to generate calculation surfaces in the model. Surfaces are individual computational domains in the orthomin matrix solver algorithm. There is a quality control system in Hydrus to find and correct any geometric object that could create errors in the finite element mesh.

4. Mesh refinements are added using the geometric feature lines (**Figure 19**). Mesh refinements are areas of smaller mesh sizes and are used primarily in source areas and other areas of sharp concentration changes to control numerical dispersion (i.e. Peclet numbers) and artifacts.
5. The finite element mesh is generated (**Figure 20**). Mesh sizes are controlled by the default mesh setting, usually 100 to 200 cm, and the mesh refinements from Step 4.
6. Lithology types are assigned to the geometric polygons based on the underlying lithology cross-section (**Figure 21**). Hydrus uses material types to define the flow and transport characteristics for each material (**Table 6**). Reference lines are added to show the location of features such as water tables. These reference lines are not used in the simulation.
7. Observation nodes are defined to obtain model results at existing monitoring well locations (**Figure 22**).
8. Pressure head and concentration initial conditions are defined for the model domain (**Figure 23**). For a calibration simulation, concentrations area always set to zero across the model domain.
   a. Hydrus initial convergence is sensitive to the initial pressure head conditions and so care must be taken to define realistic initial conditions for both the vadose and groundwater zones. Several initial pressure head configurations may be attempted to obtain a stable simulation. This is typical for a variable-saturation model because of the non-linear nature of the Richards equation (Šimůnek et al., 2012).
   b. Initial conditions can be imported from previous simulation results as applicable for a given model.
9. Boundary conditions are defined on the model boundaries (**Figure 24**). A wide range of flow and transport boundary conditions can be utilized in Hydrus. Boundary conditions can be defined on both geometric objects and the finite element mesh nodes.
10. Once a stable Hydrus model is developed (usually by small adjustments to the pressure head initial conditions), the Hydrus simulation is run and results evaluated (**Figures 25 and 26**). The calibration process then starts.

It should be noted that because of the manner in which Hydrus uses evapotranspiration and precipitation as the top boundary condition, there is no "steady-state" condition in a GAFB Hydrus vadose zone model. Water content of the vadose zone is continually changing in response to precipitation and evapotranspiration.

3.2 Model Flow Calibration

The overall model flow calibration approach will be to simulate water level changes along the model section line over time. A calibration target is an observed value or set of values which are compared to respective simulation results. A calibration variable is one that is adjusted during model calibration to improve the comparison between simulated results and observed values.

- Precipitation-related recharge is calculated by Hydrus from the precipitation and evapotranspiration meteorological input data. Temporal pond discharge and irrigation application data have been compiled and will be used to determine artificial recharge rates. Artificial recharge rates will be incorporated into a respective Hydrus model as follows:

- Recharge rates from ponds will be calculated based on discharge rates into the ponds and the evaporation rates from the ponds if discharge rate data are available or from water level changes if discharge rates are not available.
- Recharge from irrigation will be calculated internally by Hydrus from irrigation and evapotranspiration rates (Hydrus was originally developed for evaluating agricultural crops) in conjunction with data from CIMIS station 117 and associated plant coefficients. It is noted that CIMIS reference evapotranspiration (ETo) rates are for grass crops (http://www.cimis.water.ca.gov/Resources.aspx). For irrigated areas, it will generally be assumed that grass is the vegetation type and transpiration is a function of seasonal temperature changes. The guidelines in the CIMIS crop water use publication (Univ. California Cooperative Extension, 2000) will be used to estimate irrigation water losses through evaporation.
- Recharge rates will be adjusted as needed based on water level changes in nearby wells. Adjustments will be documented in the model report.
- For Hydrus models developed for sites affected by artificial recharge but away from the actual recharge area, water level changes over time will be incorporated into the respective boundary conditions based on observed water level changes at the model boundaries.

- Water level changes and associated gradient changes will be the primary model flow calibration targets. Where applicable, water level data over time will be used as transient calibration targets. Hydrus uses pressure heads and water content for the flow model output. Thus, observed water levels will be converted to pressure heads as needed.
- Primary flow calibration variables are artificial recharge rate (precipitation recharge rate is calculated by Hydrus from the meteorological input data), hydraulic conductivity, and the unsaturated van Genuchten parameters.

In general, changes in hydraulic conductivity and van Genuchten parameters in the model are made by changes in lithology. The reason is that there is a relationship between variably-saturated hydraulic conductivity and van Genuchten parameters for a given soil type as defined by the Mualem equation (Mualem, 1976). For example, it is unrealistic to have clay van Genuchten parameters and a medium sand hydraulic conductivity.

3.3 Model Transport Calibration

Vadose zone vapor and groundwater concentrations over time will be primary transport calibration targets. The model transport calibration approach will be to simulate the evolution of a contaminant plume from ground surface through the vadose zone into the Upper Aquifer with subsequent groundwater contaminant migration in the Upper Aquifer and as applicable, into the Lower Aquifer.

For transport model simulations, it is preferred to simulate plume evolution from initial release (assumed or documented) to currently observed plume extent. Otherwise, it is difficult to justify that a given transport model can reliably represent future contaminant distributions. The primary reason for this is that some transport variables, such as initial source concentration, diffusion, or decay rate, only impact simulated plume results over long periods of time (e.g. decades). For a typical Hydrus model, it is necessary to have a simulation time period of 30 to 60 years to simulate contaminant migration from initial release to recent (e.g., 2017) observed values.

Transport variables are recharge rate, hydraulic conductivity, van Genuchten parameters, porosity, bulk density, dispersion coefficient, compound distribution coefficient, vapor and water diffusion coefficients, initial source concentrations, and decay rates. As most of these parameters can be derived from site-specific geotechnical test data or literature values, the primary model transport calibration variables will be initial source concentrations and flux, dispersion coefficients, and decay rates.

Transport calibration will utilize transient (time-variable) calibration to simulated and observed concentrations. For the SS083 model, contaminant (trichloroethene) concentrations over time are shown on **Figure 27**. By using transient (time variable) calibration targets, it can be demonstrated that the model is capable of simulating plume evolution over time. Transport simulations typically address concentrations that range over several orders of magnitude so a qualitative calibration goal will be to have observed and simulated concentrations agree within approximately an order of magnitude (factor of 10) or less.

This transport calibration differs from previous modeling efforts (e.g. the OU1 Groundwater Modeling Report [MWH Americas (2007) or the OU1 Focused Feasibility Study [MWH Americas (2011)) where the observed groundwater contaminant plume concentrations were input into the models as initial conditions without generating the contaminant plume from initial conditions. The MWH model transport simulation calibration period was 10 years (from 1996 to 2006). With this type of transport calibration, it is difficult to confirm that the transport model can simulate plume development and evolution over time.

4.0 MODEL REPORT

The model report for a given Hydrus model will follow the following general outline:

1. Objective and Scope
2. Model Input Parameters
3. Model Calibration Process
   a. Flow Calibration
   b. Transport Calibration
      i. Groundwater Transport Calibration
      ii. Vapor Transport Calibration
4. Final Model Plume Calibration Results and Plume Extent
5. Model Scenarios (examples below, model scenarios are dependent on given model objectives)
   a. Example Scenario 1—Migration of residual vadose contamination to groundwater plume and defining soil/vapor remediation concentrations
   b. Example Scenario 2—Effect of diffusion from current groundwater plume into the vadose zone
   c. Example Scenario 3—Future plume migration
   d. Example Scenario 4—Remedial alternative evaluations
6. Conclusions
7. References

The model report will utilize tables and figures similar to those presented in this work plan. The goal of the report is to document the model such that inputs and results are presented in sufficient detail for regulatory agency technical peer review.

5.0 PROPOSED HYDRUS MODEL DEVELOPMENT PROCESS

Developing a variably-saturated flow and transport model has several steps that affect the overall model. Calibration of a variably-saturated model is more complex than a standard groundwater model. It is common when calibrating a groundwater model, a reasonable flow calibration does not result in an initial meaningful transport calibration. Transport calibration is where the majority of time and effort is spent in model development, particularly using transient calibration from initial conditions.

With four or five major transport calibration variables, it takes multiple simulation runs to determine the most sensitive model parameters. In addition, from experience in developing Hydrus models, it is easy to make parameter adjustments than render the model unstable or generate improbable output. Parameter adjustments must be made consistent with the underlying governing equations and realistic hydrogeologic conditions.

Since development of a variably-saturated model for GAFB involves several steps that are not included in traditional groundwater model development, it is recommended that model development progress in a cooperative manner with the various regulatory agencies and stake-holders. The following process is suggested:

1. Submittal of this work plan to solicit regulatory stakeholders' inputs on the modeling approach to meet site objectives.
2. Discussion of regulatory stakeholders' inputs in a joint working meeting and subsequent conference calls (as needed) to achieve regulatory concurrence in the modeling approach and results. The example of the SS083 model illustrated in this work plan in Sections 2 and 3 will be used as the primary discussion basis for this meeting. Development of the Hydrus model for FT082 will be a second topic.

6.0 REFERENCES

API, 2004, API Interactive LNAPL Guide, Volume 2.0.4, American Petroleum Institute, Environmental Systems & Technologies, and Aqui-Ver

Beckett, G. D., and Joy, S., 2006, Light Non-Aqueous Phase Liquid (LNAPL) Parameters Database, Downloadable Microsoft Access(r) Database: Washington, D.C., American Petroleum Institute.

Bonazountas, M., and Wagner, J., 1981, 1984, SESOIL: A Seasonal Soil Compartment Model: Arthur D. Little, Inc.

California Dept. of Water Resources, 2017, CIMIS, California Irrigation Management Information System,,: Sacramento, CA

http://www.cimis.water.ca.gov/.

CB&I Federal Services, LLC, 2017, LNAPL Conceptual Site Model Site SS030 and Source Areas ST054 and ST057, Former George Air Force Base, Victorville, California: Air Force Civil Engineer Center.

Charbeneau, R., 2007, LNAPL Distribution and Recovery Model (LDRM), Volume 1: Distribution and Recovery of Petroleum Hydrocarbon Liquids in Porous Media, API.

Charbeneau, R., and Beckett, G., 2007, LNAPL Distribution and Recovery Model (LDRM), Volume 2: User and Parameter Selection Guide, Austin, TX, API.

ESCI, 2003, SESOIL vs. VLEACH, http://www.seview.com/newsletter/vleach.html: Seview, v. 2, no. 3.

IT Corporation, Inc., 1998, Reestimation of Free Product Plume Volume and Recovery, Draft Report, Operable Unit 2, George AFB, California, AR 1271.

Johnson, P. C., 2002, Identification of Critical Parameters for the Johnson and Ettinger 1991 Vapor Intrusion Model: API.

Millington, R. J., and Quirk, J. M., 1961, Permeability of porous solids: Trans. Faraday. Soc. , v. 57, p. 1200-1207.

Mualem, Y., 1976, A New Model for Predicting the Hydraulic Conductivity of Unsaturated Porous Media: Water Resources Research, v. 12, p. 513-522.

MWH Americas, Inc., 2007, Final Groundwater Modeling Report, OU1 Optimization,. Vol. 1 and 2, AR #2195: Air Force Center for Engineering and the Environment.

-, 2011, Focused Feasibility Study OU1 TCE Groundwater Plume, plus Appendices A and B: Air Force Center for Engineering and the Environment.

Radcliff, D. E., and Šimůnek, J., 2010, Soil Physics with Hydrus Modeling and Applications, Boca Raton, FL, CRC Press.

Ravi, V., and Johnson, J. A., 1997, VLEACH A One-Dimensional Finite Difference Vadose Zone Leaching Model.

Rockware, 2017, RockWorks 17: Golden, CO, Rockware.

San Francisco Regional Water Quality Control Board, 2016, ESL - Environmental Screening Levels, Volume 2016: Oakland, CA, California Regional Water Quality Board, San Francisco Bay Region.

Šejna, M., Šimůnek, J., and Genuchten, M. T. v., 2011, User Manual, The HYDRUS Software Package for Simulating the Two- and Three-Dimensional Movement of Water, Heat, and Multiple Solutes in Variably-Saturated Porous Media: Prague, Czech Republic, PC-Progress, p. 307.

Šimůnek, J., Genuchten, M. T. v., and Šejna, M., 2012, Technical Manual, The HYDRUS Software Package for Simulating the Two- and Three-Dimensional Movement of Water, Heat, and Multiple Solutes in Variably-Saturated Porous Media: Prague, Czech Republic, PC-Progress, p. 258.

Šimůnek, J., Genuchten, M. T. v., and Šejna, M., 2016, Recent Developments and Applications of the HYDRUS Computer Software Packages: Vadose Zone Journal, v. 15, no. 8, p. 1-25.

Šimůnek, J., Jacques, D., Langergraber, G., Bradford, S. A., Šejna, M., and Genuchten, M. T. v., 2013, Numerical Modeling of Contaminant Transport Using HYDRUS and its Specialized Modules: Journal of the Indian Institute of Science, v. 93, no. 2, p. 265-284.

Univ. California Cooperative Extension, 2000, A Guide to Estimating Irrigation Water Needs of Landscape Plantings in California: California Department of Water Resources.

van Genuchten, M. T., 1980, A Closed-Form Equation for Predicting the Hydraulic Conductivity of Unsaturated Soils: Soil Science Society of America Journal,, v. 44, p. 892-898.

Yu, C., and Zheng, C., 2010, HYDRUS: Software for Flow and Transport Modeling in Variably Saturated Media: Ground Water, v. 48, no. 6, p. 787-791.

Zheng, C., and Bennett, G. D., 1995, Applied Contaminant Trasnport Modeling, New York, Van Nostrand Reinhold.

Acronyms and Abbreviations

Acronym	Reference
1-1/n	van Genuchten m (unitless)
2D	Two-dimensional
3D	Three-dimensional
α	van Genuchten curve fit alpha (1/cm)
API	American Petroleum Institute
Aptim	Aptim Federal Services LLC
CIMIS	California Irrigation Management Information System
cm	Centimeter
D^{air}	Molecular diffusion coefficient in air (cm^2/sec)
D^{eff}	Effective molecular diffusion coefficient in vapor (cm^2/sec)
D^{w}	Molecular diffusion coefficient in water (cm^2/sec)
ESL	Environmental Screen Level
GAFB	George Air Force Base
GIS	Geographical information system
H'	Unitless Henry's Law constant
h_c	Capillary pressure, pressure head for vapor-water systems (cm water)
$K(h_c)$	Hydraulic conductivity at given pressure head/water saturation (cm/d)
Koc	organic carbon partitioning coefficients
K_s	Saturated hydraulic conductivity (cm/d)
LNAPL	Light Non-Aqueous Phase Liquid
$\mu g/cm^3$	micrograms per cubic centimeter
n	van Genuchten curve fit n (unitless, referred to as the *beta* parameter in some references)
θ_T	Total porosity (fraction)
θ_v	Vapor (air)-filled porosity (fraction)
θ_v	Water-filled porosity (fraction)
S_{ew}	Effective saturation of water at given capillary pressure (fraction)
S_w	Total water saturation (fraction)
S_{wir}	irreducible water saturation (fraction)
USCS	Unified Soil Classification System
voxel	3D volumetric grid element

BACK MATERIAL BREAK

Figures

Figure 15
Plume Cross-Sections – Vertical Slice (SS083)

Figure 16
Example Time-Series Graphs

Figure 17
Hydrus Model Lithology Input and Plume Configuration (SS083)

Figure 18
Construction of Geometric Objects (SS083, Serve to Refine Finite Elements and Observation Node Locations)

Figure 19
Insert Mesh Refinements in Source Areas to Control Numerical Dispersion (SS083)

Figure 20
Construct Finite Element Mesh (SS083)

Figure 21
Define Lithology Using Geometric Objects (SS083)

Figure 22
Define Observation Nodes at Well Locations (SS083)

Figure 23
Define Initial Conditions (SS083)

Figure 24
Define Boundary Conditions (SS083)

Figure 25
Pressure Head Results (SS083)

Figure 26
40-year TCE Simulation Results (SS083, 1965 – 2005)

Figure 27
Example Transient Transport Calibration Graphs for SS083

BACK MATERIAL BREAK

Tables